N-DESMETHYLCLOMIPRAMINE AC.

Other names: Clomipramine M(Nor), acetylated
Inchi: InChI=1S/C20H23ClN2O/c1-15(24)22(2)12-5-13-23-19-7-4-3-6-16(19)8-9-17-10-11-18(2
InchiKey: MKZYWCOSALTCPB-UHFFFAOYSA-N
Formula: C20H23ClN2O
SMILES: CC(=O)N(C)CCCN1c2ccccc2CCc2ccc(Cl)cc21
Mol. weight [g/mol]: 342.87

Physical Properties

Property code	Value	Unit	Source
ie	7.38	eV	Cheméo Relay (1.0)
log10ws	-4.51		Cheméo Relay (1.0)
logp	4.445		Crippen Method
mcvol	268.050	ml/mol	McGowan Method
rinpol	2994.00		NIST Webbook
rinpol	2994.00		NIST Webbook
tf	380.74	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72103492&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point